Clinochlore [$Mg_3(Mg_2Al)(Si_3Al)O_{10}(OH)_8$, $S5_5$] Structure: A3B5C4D2_mC112_15_a3ef_5f_4f_2f-001

This structure previously used the label(s) `A3B5C4D2_mC112_15_a3ef_5f_4f_2f`. Calls to these addresses will be redirected here.

Cite this page as:

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- D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

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https://aflow.org/prototype-encyclopedia/RDRH

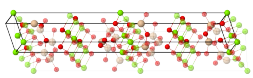
https://aflow.org/prototype-encyclopedia/A3B5C4D2_mC112_15_a3ef_5f_4f_2f-001

Prototype	$Mg_3O_5(OH)_4Si_2$
AFLOW prototype label	A3B5C4D2_mC112_15_a3ef_5f_4f_2f-001
***Strukturbericht* designation**	$S5_5$
Mineral name	clinochlore
ICSD	26850
CCDC	1602229
Pearson symbol	mC112
Space group number	15
Space group symbol	$C2/c$
AFLOW prototype command	`aflow --proto=A3B5C4D2_mC112_15_a3ef_5f_4f_2f-001 --params=`$a, b/a, c/a, \beta, y_2, y_3, y_4, x_5, y_5, z_5, x_6, y_6, z_6, x_7, y_7, z_7, x_8, y_8, z_8, x_9, y_9, z_9, x_{10}, y_{10}, z_{10}, x_{11}, y_{11}, z_{11}, x_{12}, y_{12}, z_{12}, x_{13}, y_{13}, z_{13}, x_{14}, y_{14}, z_{14}, x_{15}, y_{15}, z_{15}, x_{16}, y_{16}, z_{16}$

- We follow the interpretation of (McMurchy, 1934) as given by (Downs, 2003): We have labeled "Mg (4e)" are actually 2/3 magnesium and 1/3 aluminum, and the sites we have labeled "Si (8f)" are 3/4 silicon and 1/4 aluminum. This does not exactly match the ICSD entry.

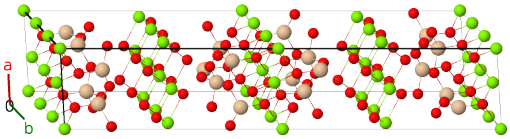
Base-centered Monoclinic primitive vectors

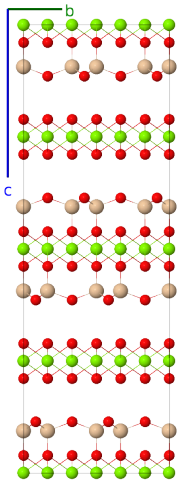
$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{1}{2}b\,\hat{\mathbf{y}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\cos\beta\,\hat{\mathbf{x}} + c\sin\beta\,\hat{\mathbf{z}}$$

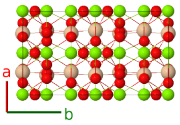


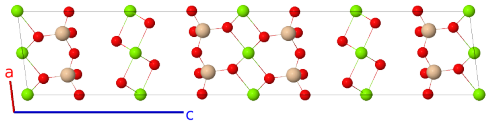
Basis vectors

Mg
O
Si









		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(4a)	Mg I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}c\cos\beta\,\hat{\mathbf{x}} + \frac{1}{2}c\sin\beta\,\hat{\mathbf{z}}$	(4a)	Mg I
$\mathbf{B_3}$	=	$-y_2\,\mathbf{a}_1 + y_2\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}c\cos\beta\,\hat{\mathbf{x}} + by_2\,\hat{\mathbf{y}} + \frac{1}{4}c\sin\beta\,\hat{\mathbf{z}}$	(4e)	Mg II
$\mathbf{B_4}$	=	$y_2\,\mathbf{a}_1 - y_2\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{3}{4}c\cos\beta\,\hat{\mathbf{x}} - by_2\,\hat{\mathbf{y}} + \frac{3}{4}c\sin\beta\,\hat{\mathbf{z}}$	(4e)	Mg II
$\mathbf{B_5}$	=	$-y_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}c\cos\beta\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} + \frac{1}{4}c\sin\beta\,\hat{\mathbf{z}}$	(4e)	Mg III
$\mathbf{B_6}$	=	$y_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{3}{4}c\cos\beta\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} + \frac{3}{4}c\sin\beta\,\hat{\mathbf{z}}$	(4e)	Mg III
$\mathbf{B_7}$	=	$-y_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}c\cos\beta\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} + \frac{1}{4}c\sin\beta\,\hat{\mathbf{z}}$	(4e)	Mg IV
$\mathbf{B_8}$	=	$y_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{3}{4}c\cos\beta\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} + \frac{3}{4}c\sin\beta\,\hat{\mathbf{z}}$	(4e)	Mg IV
$\mathbf{B_9}$	=	$(x_5 - y_5)\,\mathbf{a}_1 + (x_5 + y_5)\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$(ax_5 + cz_5\cos\beta)\,\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}} + cz_5\sin\beta\,\hat{\mathbf{z}}$	(8f)	Mg V
$\mathbf{B_{10}}$	=	$-(x_5 + y_5)\,\mathbf{a}_1 - (x_5 - y_5)\,\mathbf{a}_2 - \left(z_5 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\left(ax_5 + c\left(z_5 - \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}} - c\left(z_5 - \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(8f)	Mg V
$\mathbf{B_{11}}$	=	$-(x_5 - y_5)\,\mathbf{a}_1 - (x_5 + y_5)\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$-(ax_5 + cz_5\cos\beta)\,\hat{\mathbf{x}} - by_5\,\hat{\mathbf{y}} - cz_5\sin\beta\,\hat{\mathbf{z}}$	(8f)	Mg V
$\mathbf{B_{12}}$	=	$(x_5 + y_5)\,\mathbf{a}_1 + (x_5 - y_5)\,\mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_5 + c\left(z_5 + \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - by_5\,\hat{\mathbf{y}} + c\left(z_5 + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(8f)	Mg V
$\mathbf{B_{13}}$	=	$(x_6 - y_6)\,\mathbf{a}_1 + (x_6 + y_6)\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$(ax_6 + cz_6\cos\beta)\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} + cz_6\sin\beta\,\hat{\mathbf{z}}$	(8f)	O I
$\mathbf{B_{14}}$	=	$-(x_6 + y_6)\,\mathbf{a}_1 - (x_6 - y_6)\,\mathbf{a}_2 - \left(z_6 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\left(ax_6 + c\left(z_6 - \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} - c\left(z_6 - \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(8f)	O I
$\mathbf{B_{15}}$	=	$-(x_6 - y_6)\,\mathbf{a}_1 - (x_6 + y_6)\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$	=	$-(ax_6 + cz_6\cos\beta)\,\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} - cz_6\sin\beta\,\hat{\mathbf{z}}$	(8f)	O I
$\mathbf{B_{16}}$	=	$(x_6 + y_6)\,\mathbf{a}_1 + (x_6 - y_6)\,\mathbf{a}_2 + \left(z_6 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_6 + c\left(z_6 + \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} + c\left(z_6 + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(8f)	O I
$\mathbf{B_{17}}$	=	$(x_7 - y_7)\,\mathbf{a}_1 + (x_7 + y_7)\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$(ax_7 + cz_7\cos\beta)\,\hat{\mathbf{x}} + by_7\,\hat{\mathbf{y}} + cz_7\sin\beta\,\hat{\mathbf{z}}$	(8f)	O II
$\mathbf{B_{18}}$	=	$-(x_7 + y_7)\,\mathbf{a}_1 - (x_7 - y_7)\,\mathbf{a}_2 - \left(z_7 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\left(ax_7 + c\left(z_7 - \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + by_7\,\hat{\mathbf{y}} - c\left(z_7 - \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(8f)	O II
$\mathbf{B_{19}}$	=	$-(x_7 - y_7)\,\mathbf{a}_1 - (x_7 + y_7)\,\mathbf{a}_2 - z_7\,\mathbf{a}_3$	=	$-(ax_7 + cz_7\cos\beta)\,\hat{\mathbf{x}} - by_7\,\hat{\mathbf{y}} - cz_7\sin\beta\,\hat{\mathbf{z}}$	(8f)	O II
$\mathbf{B_{20}}$	=	$(x_7 + y_7)\,\mathbf{a}_1 + (x_7 - y_7)\,\mathbf{a}_2 + \left(z_7 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_7 + c\left(z_7 + \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - by_7\,\hat{\mathbf{y}} + c\left(z_7 + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(8f)	O II
$\mathbf{B_{21}}$	=	$(x_8 - y_8)\,\mathbf{a}_1 + (x_8 + y_8)\,\mathbf{a}_2 + z_8\,\mathbf{a}_3$	=	$(ax_8 + cz_8\cos\beta)\,\hat{\mathbf{x}} + by_8\,\hat{\mathbf{y}} + cz_8\sin\beta\,\hat{\mathbf{z}}$	(8f)	O III
$\mathbf{B_{22}}$	=	$-(x_8 + y_8)\,\mathbf{a}_1 - (x_8 - y_8)\,\mathbf{a}_2 - \left(z_8 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\left(ax_8 + c\left(z_8 - \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + by_8\,\hat{\mathbf{y}} - c\left(z_8 - \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(8f)	O III
$\mathbf{B_{23}}$	=	$-(x_8 - y_8)\,\mathbf{a}_1 - (x_8 + y_8)\,\mathbf{a}_2 - z_8\,\mathbf{a}_3$	=	$-(ax_8 + cz_8\cos\beta)\,\hat{\mathbf{x}} - by_8\,\hat{\mathbf{y}} - cz_8\sin\beta\,\hat{\mathbf{z}}$	(8f)	O III
$\mathbf{B_{24}}$	=	$(x_8 + y_8)\,\mathbf{a}_1 + (x_8 - y_8)\,\mathbf{a}_2 + \left(z_8 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_8 + c\left(z_8 + \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - by_8\,\hat{\mathbf{y}} + c\left(z_8 + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(8f)	O III
$\mathbf{B_{25}}$	=	$(x_9 - y_9)\,\mathbf{a}_1 + (x_9 + y_9)\,\mathbf{a}_2 + z_9\,\mathbf{a}_3$	=	$(ax_9 + cz_9\cos\beta)\,\hat{\mathbf{x}} + by_9\,\hat{\mathbf{y}} + cz_9\sin\beta\,\hat{\mathbf{z}}$	(8f)	O IV
$\mathbf{B_{26}}$	=	$-(x_9 + y_9)\,\mathbf{a}_1 - (x_9 - y_9)\,\mathbf{a}_2 - \left(z_9 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\left(ax_9 + c\left(z_9 - \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + by_9\,\hat{\mathbf{y}} - c\left(z_9 - \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(8f)	O IV

$$\mathbf{B_{27}} = -(x_9 - y_9)\,\mathbf{a}_1 - (x_9 + y_9)\,\mathbf{a}_2 - z_9\,\mathbf{a}_3 = -(ax_9 + cz_9\cos\beta)\,\hat{\mathbf{x}} - by_9\,\hat{\mathbf{y}} - cz_9\sin\beta\,\hat{\mathbf{z}} \quad (8f) \quad \text{O IV}$$

$$\mathbf{B_{28}} = (x_9 + y_9)\,\mathbf{a}_1 + (x_9 - y_9)\,\mathbf{a}_2 + \left(z_9 + \tfrac{1}{2}\right)\mathbf{a}_3 = \left(ax_9 + c\left(z_9 + \tfrac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - by_9\,\hat{\mathbf{y}} + c\left(z_9 + \tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}} \quad (8f) \quad \text{O IV}$$

$$\mathbf{B_{29}} = (x_{10} - y_{10})\,\mathbf{a}_1 + (x_{10} + y_{10})\,\mathbf{a}_2 + z_{10}\,\mathbf{a}_3 = (ax_{10} + cz_{10}\cos\beta)\,\hat{\mathbf{x}} + by_{10}\,\hat{\mathbf{y}} + cz_{10}\sin\beta\,\hat{\mathbf{z}} \quad (8f) \quad \text{O V}$$

$$\mathbf{B_{30}} = -(x_{10} + y_{10})\,\mathbf{a}_1 - (x_{10} - y_{10})\,\mathbf{a}_2 - \left(z_{10} - \tfrac{1}{2}\right)\mathbf{a}_3 = -\left(ax_{10} + c\left(z_{10} - \tfrac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + by_{10}\,\hat{\mathbf{y}} - c\left(z_{10} - \tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}} \quad (8f) \quad \text{O V}$$

$$\mathbf{B_{31}} = -(x_{10} - y_{10})\,\mathbf{a}_1 - (x_{10} + y_{10})\,\mathbf{a}_2 - z_{10}\,\mathbf{a}_3 = -(ax_{10} + cz_{10}\cos\beta)\,\hat{\mathbf{x}} - by_{10}\,\hat{\mathbf{y}} - cz_{10}\sin\beta\,\hat{\mathbf{z}} \quad (8f) \quad \text{O V}$$

$$\mathbf{B_{32}} = (x_{10} + y_{10})\,\mathbf{a}_1 + (x_{10} - y_{10})\,\mathbf{a}_2 + \left(z_{10} + \tfrac{1}{2}\right)\mathbf{a}_3 = \left(ax_{10} + c\left(z_{10} + \tfrac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - by_{10}\,\hat{\mathbf{y}} + c\left(z_{10} + \tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}} \quad (8f) \quad \text{O V}$$

$$\mathbf{B_{33}} = (x_{11} - y_{11})\,\mathbf{a}_1 + (x_{11} + y_{11})\,\mathbf{a}_2 + z_{11}\,\mathbf{a}_3 = (ax_{11} + cz_{11}\cos\beta)\,\hat{\mathbf{x}} + by_{11}\,\hat{\mathbf{y}} + cz_{11}\sin\beta\,\hat{\mathbf{z}} \quad (8f) \quad \text{OH I}$$

$$\mathbf{B_{34}} = -(x_{11} + y_{11})\,\mathbf{a}_1 - (x_{11} - y_{11})\,\mathbf{a}_2 - \left(z_{11} - \tfrac{1}{2}\right)\mathbf{a}_3 = -\left(ax_{11} + c\left(z_{11} - \tfrac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + by_{11}\,\hat{\mathbf{y}} - c\left(z_{11} - \tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}} \quad (8f) \quad \text{OH I}$$

$$\mathbf{B_{35}} = -(x_{11} - y_{11})\,\mathbf{a}_1 - (x_{11} + y_{11})\,\mathbf{a}_2 - z_{11}\,\mathbf{a}_3 = -(ax_{11} + cz_{11}\cos\beta)\,\hat{\mathbf{x}} - by_{11}\,\hat{\mathbf{y}} - cz_{11}\sin\beta\,\hat{\mathbf{z}} \quad (8f) \quad \text{OH I}$$

$$\mathbf{B_{36}} = (x_{11} + y_{11})\,\mathbf{a}_1 + (x_{11} - y_{11})\,\mathbf{a}_2 + \left(z_{11} + \tfrac{1}{2}\right)\mathbf{a}_3 = \left(ax_{11} + c\left(z_{11} + \tfrac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - by_{11}\,\hat{\mathbf{y}} + c\left(z_{11} + \tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}} \quad (8f) \quad \text{OH I}$$

$$\mathbf{B_{37}} = (x_{12} - y_{12})\,\mathbf{a}_1 + (x_{12} + y_{12})\,\mathbf{a}_2 + z_{12}\,\mathbf{a}_3 = (ax_{12} + cz_{12}\cos\beta)\,\hat{\mathbf{x}} + by_{12}\,\hat{\mathbf{y}} + cz_{12}\sin\beta\,\hat{\mathbf{z}} \quad (8f) \quad \text{OH II}$$

$$\mathbf{B_{38}} = -(x_{12} + y_{12})\,\mathbf{a}_1 - (x_{12} - y_{12})\,\mathbf{a}_2 - \left(z_{12} - \tfrac{1}{2}\right)\mathbf{a}_3 = -\left(ax_{12} + c\left(z_{12} - \tfrac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + by_{12}\,\hat{\mathbf{y}} - c\left(z_{12} - \tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}} \quad (8f) \quad \text{OH II}$$

$$\mathbf{B_{39}} = -(x_{12} - y_{12})\,\mathbf{a}_1 - (x_{12} + y_{12})\,\mathbf{a}_2 - z_{12}\,\mathbf{a}_3 = -(ax_{12} + cz_{12}\cos\beta)\,\hat{\mathbf{x}} - by_{12}\,\hat{\mathbf{y}} - cz_{12}\sin\beta\,\hat{\mathbf{z}} \quad (8f) \quad \text{OH II}$$

$$\mathbf{B_{40}} = (x_{12} + y_{12})\,\mathbf{a}_1 + (x_{12} - y_{12})\,\mathbf{a}_2 + \left(z_{12} + \tfrac{1}{2}\right)\mathbf{a}_3 = \left(ax_{12} + c\left(z_{12} + \tfrac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - by_{12}\,\hat{\mathbf{y}} + c\left(z_{12} + \tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}} \quad (8f) \quad \text{OH II}$$

$$\mathbf{B_{41}} = (x_{13} - y_{13})\,\mathbf{a}_1 + (x_{13} + y_{13})\,\mathbf{a}_2 + z_{13}\,\mathbf{a}_3 = (ax_{13} + cz_{13}\cos\beta)\,\hat{\mathbf{x}} + by_{13}\,\hat{\mathbf{y}} + cz_{13}\sin\beta\,\hat{\mathbf{z}} \quad (8f) \quad \text{OH III}$$

$$\mathbf{B_{42}} = -(x_{13} + y_{13})\,\mathbf{a}_1 - (x_{13} - y_{13})\,\mathbf{a}_2 - \left(z_{13} - \tfrac{1}{2}\right)\mathbf{a}_3 = -\left(ax_{13} + c\left(z_{13} - \tfrac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + by_{13}\,\hat{\mathbf{y}} - c\left(z_{13} - \tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}} \quad (8f) \quad \text{OH III}$$

$$\mathbf{B_{43}} = -(x_{13} - y_{13})\,\mathbf{a}_1 - (x_{13} + y_{13})\,\mathbf{a}_2 - z_{13}\,\mathbf{a}_3 = -(ax_{13} + cz_{13}\cos\beta)\,\hat{\mathbf{x}} - by_{13}\,\hat{\mathbf{y}} - cz_{13}\sin\beta\,\hat{\mathbf{z}} \quad (8f) \quad \text{OH III}$$

$$\mathbf{B_{44}} = (x_{13} + y_{13})\,\mathbf{a}_1 + (x_{13} - y_{13})\,\mathbf{a}_2 + \left(z_{13} + \tfrac{1}{2}\right)\mathbf{a}_3 = \left(ax_{13} + c\left(z_{13} + \tfrac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - by_{13}\,\hat{\mathbf{y}} + c\left(z_{13} + \tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}} \quad (8f) \quad \text{OH III}$$

$$\mathbf{B_{45}} = (x_{14} - y_{14})\,\mathbf{a}_1 + (x_{14} + y_{14})\,\mathbf{a}_2 + z_{14}\,\mathbf{a}_3 = (ax_{14} + cz_{14}\cos\beta)\,\hat{\mathbf{x}} + by_{14}\,\hat{\mathbf{y}} + cz_{14}\sin\beta\,\hat{\mathbf{z}} \quad (8f) \quad \text{OH IV}$$

$$\mathbf{B_{46}} = -(x_{14} + y_{14})\,\mathbf{a}_1 - (x_{14} - y_{14})\,\mathbf{a}_2 - \left(z_{14} - \tfrac{1}{2}\right)\mathbf{a}_3 = -\left(ax_{14} + c\left(z_{14} - \tfrac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + by_{14}\,\hat{\mathbf{y}} - c\left(z_{14} - \tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}} \quad (8f) \quad \text{OH IV}$$

$$\mathbf{B_{47}} = -(x_{14} - y_{14})\,\mathbf{a}_1 - (x_{14} + y_{14})\,\mathbf{a}_2 - z_{14}\,\mathbf{a}_3 = -(ax_{14} + cz_{14}\cos\beta)\,\hat{\mathbf{x}} - by_{14}\,\hat{\mathbf{y}} - cz_{14}\sin\beta\,\hat{\mathbf{z}} \quad (8f) \quad \text{OH IV}$$

$$\mathbf{B_{48}} = (x_{14} + y_{14})\,\mathbf{a}_1 + (x_{14} - y_{14})\,\mathbf{a}_2 + \left(z_{14} + \tfrac{1}{2}\right)\mathbf{a}_3 = \left(ax_{14} + c\left(z_{14} + \tfrac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - by_{14}\,\hat{\mathbf{y}} + c\left(z_{14} + \tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}} \quad (8f) \quad \text{OH IV}$$

$$\mathbf{B_{49}} = (x_{15} - y_{15})\,\mathbf{a}_1 + (x_{15} + y_{15})\,\mathbf{a}_2 + z_{15}\,\mathbf{a}_3 = (ax_{15} + cz_{15}\cos\beta)\,\hat{\mathbf{x}} + by_{15}\,\hat{\mathbf{y}} + cz_{15}\sin\beta\,\hat{\mathbf{z}} \quad (8f) \quad \text{Si I}$$

$\mathbf{B_{50}}$	$=$	$-\left(x_{15}+y_{15}\right)\,\mathbf{a}_1 - \left(x_{15}-y_{15}\right)\,\mathbf{a}_2 - \left(z_{15}-\frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$-\left(ax_{15}+c\left(z_{15}-\frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + by_{15}\,\hat{\mathbf{y}} - c\left(z_{15}-\frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(8f)	Si I
$\mathbf{B_{51}}$	$=$	$-\left(x_{15}-y_{15}\right)\,\mathbf{a}_1 - \left(x_{15}+y_{15}\right)\,\mathbf{a}_2 - z_{15}\,\mathbf{a}_3$	$=$	$-\left(ax_{15}+cz_{15}\cos\beta\right)\,\hat{\mathbf{x}} - by_{15}\,\hat{\mathbf{y}} - cz_{15}\sin\beta\,\hat{\mathbf{z}}$	(8f)	Si I
$\mathbf{B_{52}}$	$=$	$\left(x_{15}+y_{15}\right)\,\mathbf{a}_1 + \left(x_{15}-y_{15}\right)\,\mathbf{a}_2 + \left(z_{15}+\frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$\left(ax_{15}+c\left(z_{15}+\frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - by_{15}\,\hat{\mathbf{y}} + c\left(z_{15}+\frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(8f)	Si I
$\mathbf{B_{53}}$	$=$	$\left(x_{16}-y_{16}\right)\,\mathbf{a}_1 + \left(x_{16}+y_{16}\right)\,\mathbf{a}_2 + z_{16}\,\mathbf{a}_3$	$=$	$\left(ax_{16}+cz_{16}\cos\beta\right)\,\hat{\mathbf{x}} + by_{16}\,\hat{\mathbf{y}} + cz_{16}\sin\beta\,\hat{\mathbf{z}}$	(8f)	Si II
$\mathbf{B_{54}}$	$=$	$-\left(x_{16}+y_{16}\right)\,\mathbf{a}_1 - \left(x_{16}-y_{16}\right)\,\mathbf{a}_2 - \left(z_{16}-\frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$-\left(ax_{16}+c\left(z_{16}-\frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + by_{16}\,\hat{\mathbf{y}} - c\left(z_{16}-\frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(8f)	Si II
$\mathbf{B_{55}}$	$=$	$-\left(x_{16}-y_{16}\right)\,\mathbf{a}_1 - \left(x_{16}+y_{16}\right)\,\mathbf{a}_2 - z_{16}\,\mathbf{a}_3$	$=$	$-\left(ax_{16}+cz_{16}\cos\beta\right)\,\hat{\mathbf{x}} - by_{16}\,\hat{\mathbf{y}} - cz_{16}\sin\beta\,\hat{\mathbf{z}}$	(8f)	Si II
$\mathbf{B_{56}}$	$=$	$\left(x_{16}+y_{16}\right)\,\mathbf{a}_1 + \left(x_{16}-y_{16}\right)\,\mathbf{a}_2 + \left(z_{16}+\frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$\left(ax_{16}+c\left(z_{16}+\frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - by_{16}\,\hat{\mathbf{y}} + c\left(z_{16}+\frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(8f)	Si II

References

[1] R. C. McMurchy, *The Crystal Structure of the Chlorite Minerals*, Z. Kristallogr. **88**, 420–432 (1934), doi:10.1524/zkri.1934.88.1.420.

Found in

[1] R. T. Downs and M. Hall-Wallace, *The American Mineralogist Crystal Structure Database*, Am. Mineral. **88**, 247–250 (2003).

First cited in

D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.